

The Jahn-Teller effect in Cr⁵⁺-doped PbTiO₃: A multi-frequency electron paramagnetic resonance study

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Abstract

Electron paramagnetic resonance (EPR) spectra of Cr⁵⁺ defects incorporated on Ti⁴⁺ sites in powdered ceramics of PbTiO₃ were investigated in the temperature range 50-400K at 9GHz (X), 34GHz (Q) and 94GHz (W band). The Jahn-Teller effect stabilizes the vibronic ground state of the 3d¹ electron of the Cr⁵⁺ ion and leads to a tetragonally distorted defect- O₆ octahedron with the point symmetry D_{4h}. The spontaneous electrical polarization present in the ferroelectric phase of PbTiO₃ appears as a further perturbation producing an additional g-tensor contribution by the quadratic field effect. Its symmetry is dependent on the orientation of the electrical polarization with respect to the Jahn-Teller distortion axis, the tetragonal axis of the defect- O₆ octahedron. If the polarization of a domain is anti-or parallel to this axis, the local tetragonal symmetry of the Cr⁵⁺ ion persists whereas it is reduced by a perpendicular orientation. Anisotropic EPR spectra of tetragonally and orthorhombic distorted Cr⁵⁺O₆¹²⁻ are detected at low temperatures. Increasing the temperature, the peaks of the two spectra are broadened and a motionally averaged isotropic spectrum appears at 200K. © 2010 IOP Publishing Ltd.

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